WE CLAIM:

1. A crystal of BTK kinase domain having a space group symmetry of $P2_12_12_1$ and comprising a unit cell having the dimensions of *a, b,* and *c*, where *a* is about 45 Å, *b* is about 104 Å, and *c* is about 116 Å.

2. The crystal of claim 1, having an amino acid sequence of SEQ ID NO:4.

3. A molecule or molecular complex comprising at least a portion of the BTK kinase domain binding pocket, wherein the binding pocket comprises the amino acids listed in Table 2, the binding pocket defined by a set of points having a root mean square deviation of less than about 0.70 Å from points representing the backbone atoms of said amino acids as represented by the structure coordinates listed in Table 1.

4. A scalable three-dimensional configuration of points, at least a portion of said points derived from structure coordinates listed in Table 1, comprising a BTK kinase domain binding pocket, wherein the BTK kinase domain forms a crystal having the space group symmetry $P2_12_12_1$.

5. The scalable three-dimensional configuration of points of claim 4, wherein substantially all of the points are derived from structure coordinates listed in Table 1.

6. The scalable three-dimensional configuration of points of claim 4, wherein at least a portion of the points are derived from structure coordinates representing locations of at least the backbone atoms of amino acids defining the BTK kinase domain binding pocket.

7. The scalable three-dimensional configuration of points of claim 4, wherein the binding pocket comprises the amino acids listed in Table 2.

8. A scalable three-dimensional configuration of points displayed as a holographic image, a stereodiagram, a model, or a computer-displayed image, at least

a portion of said points derived from structure coordinates listed in Table 1, comprising a BTK kinase domain binding pocket, wherein the BTK kinase domain forms a crystal having the space group symmetry $P2_12_12_1$.

9. A machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein a machine programmed with instructions for using such data displays a graphical three-dimensional representation of at least one molecule or molecular complex comprising at least a portion of a BTK kinase domain binding pocket, the binding pocket defined by a set of points having a root mean square deviation of less than about 0.05 Å from points representing the atoms of said amino acids as represented by the structure coordinates listed in Table 1.

10. A machine readable data storage medium comprising data storage material encoded with a first set of machine readable data which is combined with a second set of machine readable data using a machine programmed with instructions for using said first and second sets of data, determines at least a portion of the structure coordinates corresponding to the second set of data, wherein the first set of data comprises a Fourier transform of at least a portion of the BTK kinase domain structural coordinates of Table 1, and wherein the second set of data comprises an X-ray diffraction pattern of an unknown molecule or molecular complex.

11. A method for obtaining structural information about a molecule or molecular complex comprising application of at least a portion of the BTK kinase domain structure coordinates of Table 1 to an X-ray diffraction pattern of the molecule or molecular complex's crystal structure to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex.

12. A computer-assisted method for identifying an agent that modulates BTK activity comprising:

(a) providing a computer modeling application with a set of structure coordinates of Table 1 defining at least a portion of a BTK kinase domain;

(b) providing the computer modeling application with a set of structure coordinates for a test compound; and

(c) modeling the structure of (a) complexed with (b) to determine if the test compound binds to the BTK kinase domain binding pocket.

13. The method of claim 12, where the binding pocket comprises the amino acids listed in Table 2.

14. A computer-assisted method for designing a compound that binds the BTK kinase domain binding pocket, comprising:

(a) providing a computer modeling application with a set of structural coordinates of Table 1 defining at least a portion of the BTK kinase domain; and

(b) modeling the structural coordinates of (a) to determine a complementary molecule that binds the BTK kinase domain pocket.

15. A molecular complex comprising a BTK kinase domain binding pocket defined by at least a portion of the structural coordinates of Table 1 complexed with a compound having complementarity to at least a portion of the structural coordinates of Table 1.